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DESIGN OF FEASIBLE BLENDS OF GASOLINE AND BIOFUELS USING A SYSTEMATIC COMPUTER AIDED TECHNIQUE

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BY:
NOR ALAFIZA YUNUS

Outline

- Introduction
- Motivation
- Objective
- Methodology
- Results
- Future work

Introduction

Chemical Product Design

FA: Forward approach

Specify the structures

Structure of molecules / process flow sheets

Determine the structures that match the target

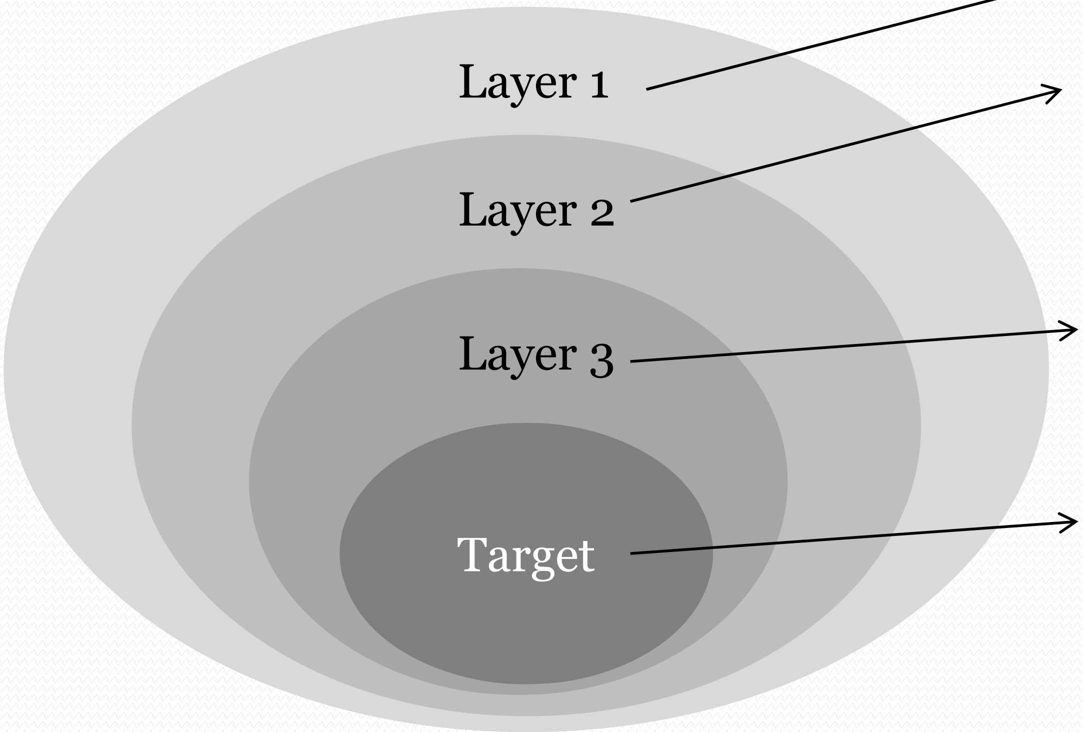
Use property or behavior models

Set of target (desired) properties

RA: Reverse approach

Specify the properties

Introduction



- Layer 1: Start searching at bigger space
- Layer 2: Reduce searching space when a constraint was introduce – eliminate unwanted candidates
- Layer 3: Further reduce searching space when more constraints were introduce
- Target area: Finally, the right candidate was able to find at a small target area

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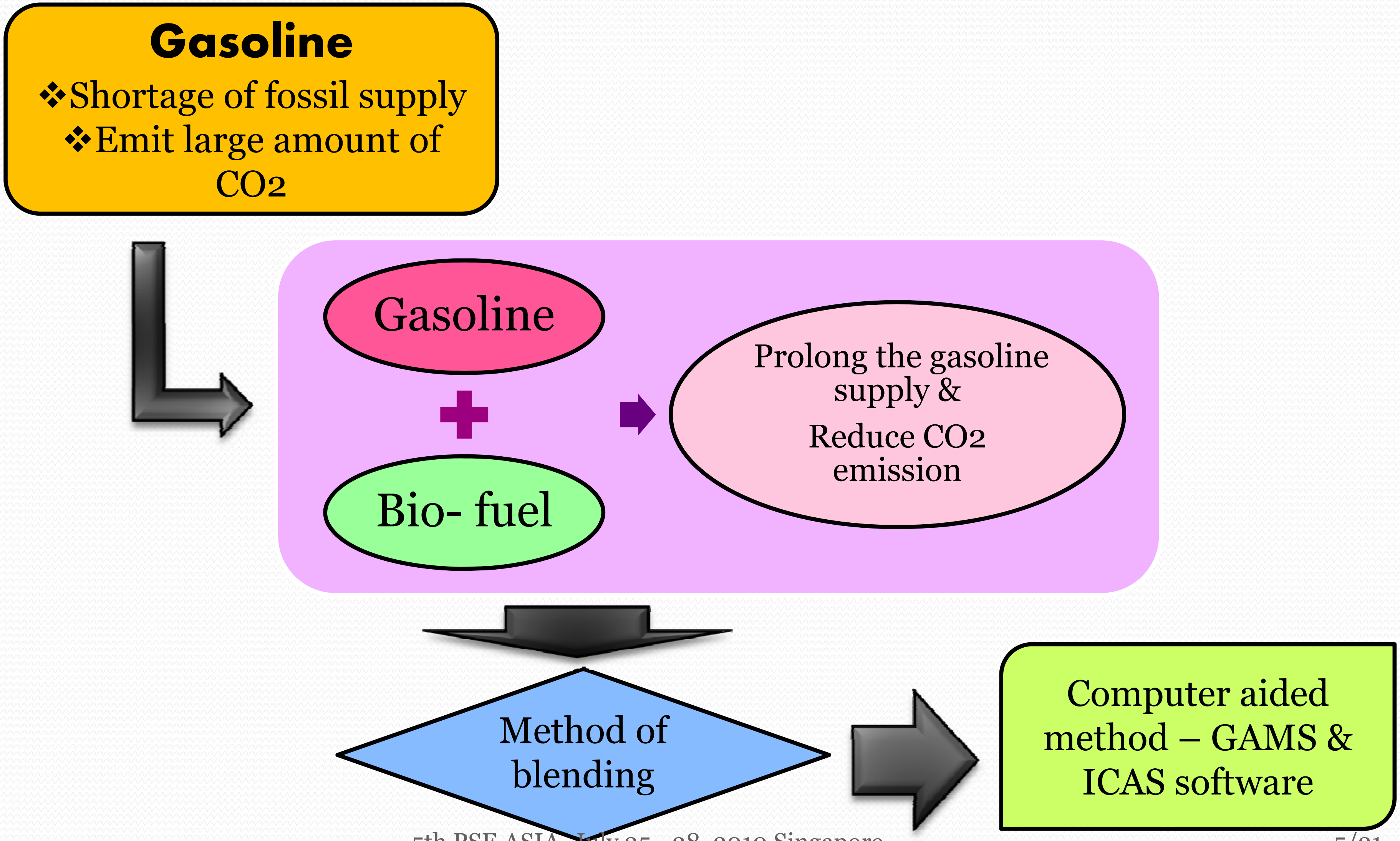
Motivation



Objective

To find a set of feasible blend of gasoline and bio-fuel which are could reduce fossil fuel consumption using a systematic computer aided approach

Methodology

Step 1 — Identify target properties and target values

Step 2 — Identify properties model

Step 3 — Identify the possible blend mixture

Step 4 — Generate the possible blend candidates

Step 5 — Validate the model

Methodology

step	Task	Method & tools	Output
1	Identify the important target property	Literature (journals) Blending guideline	List of target properties
	Set the target value for each target property	Literature (journals), Blending regulation Existing product	List of constraints
2	Identify pure and mixture property model	Literature, calculated directly from chemical structure	Pure property models Mixture property models
3	Identify the feasible mixture	ICAS	List of feasible blend compositions
4	Generate the possible mixture candidates	GAMS	List of several possible mixture candidates
5	Model validation	Experiment	Experimental data

ICAS: Integrated Computer Aided System

Methodology

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Property	Target value
Heating Value	> 35 MJ/kg
Octane number	> 90
Density	700 – 790 kg/m^3
Kinematic viscosity	< 2.41 mm^2/s

Methodology

- Step 1: Identify target properties and target values
- Step 2: Identify properties model
- Step 3: Identify the possible blend mixture
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Property	Model
Heating Value	$HV_{mix} = \sum x_i HV_i$
Octane number	$ON = \sum x_i ON_i$
Density	$\rho_{mix} = \sum x_i \rho_i$
Kinematic viscosity	$\nu_{mix} = \frac{1}{\rho_{mix}} \exp\left(\sum \upsilon_i \ln \eta_i\right)$

Methodology

- Step 1 — Identify target properties and target values
- Step 2 — Identify properties model
- **Step 3 — Identify the possible blend mixture**
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PT-flash (multiphase) calculation

Thermodynamic model

Soave-Redlich-Kwong

Methodology

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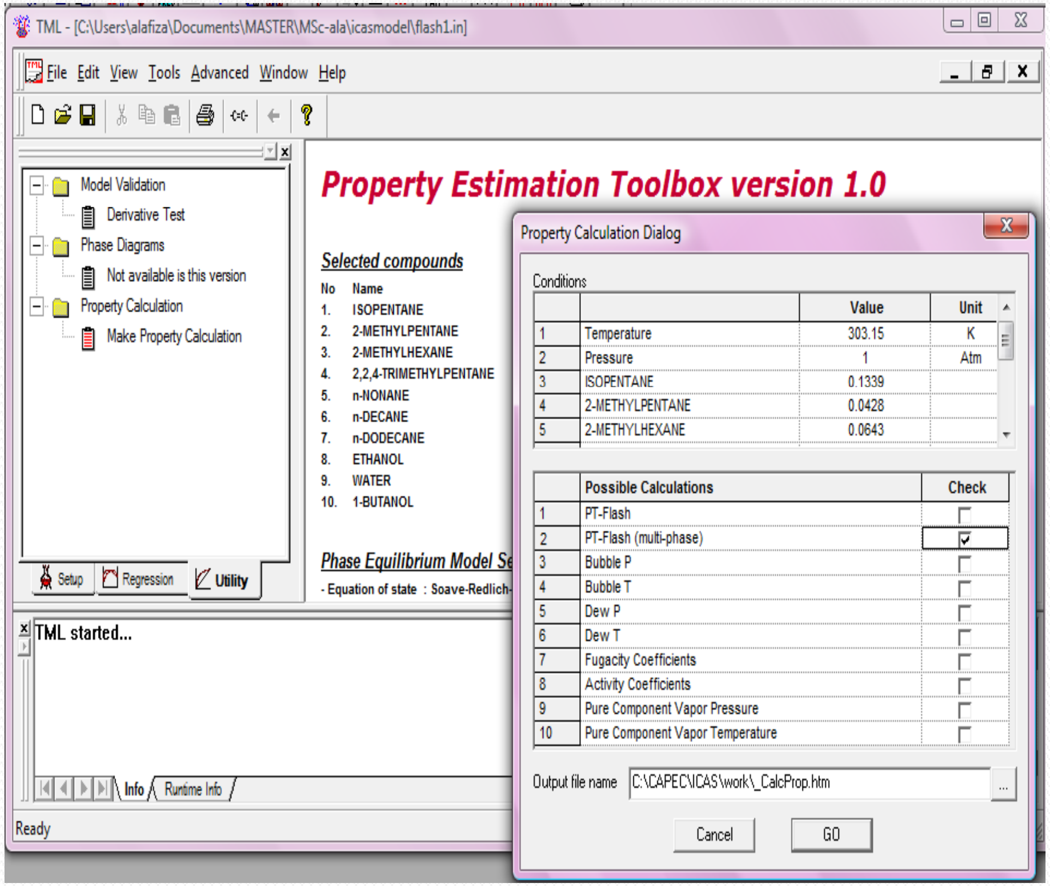

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Methodology

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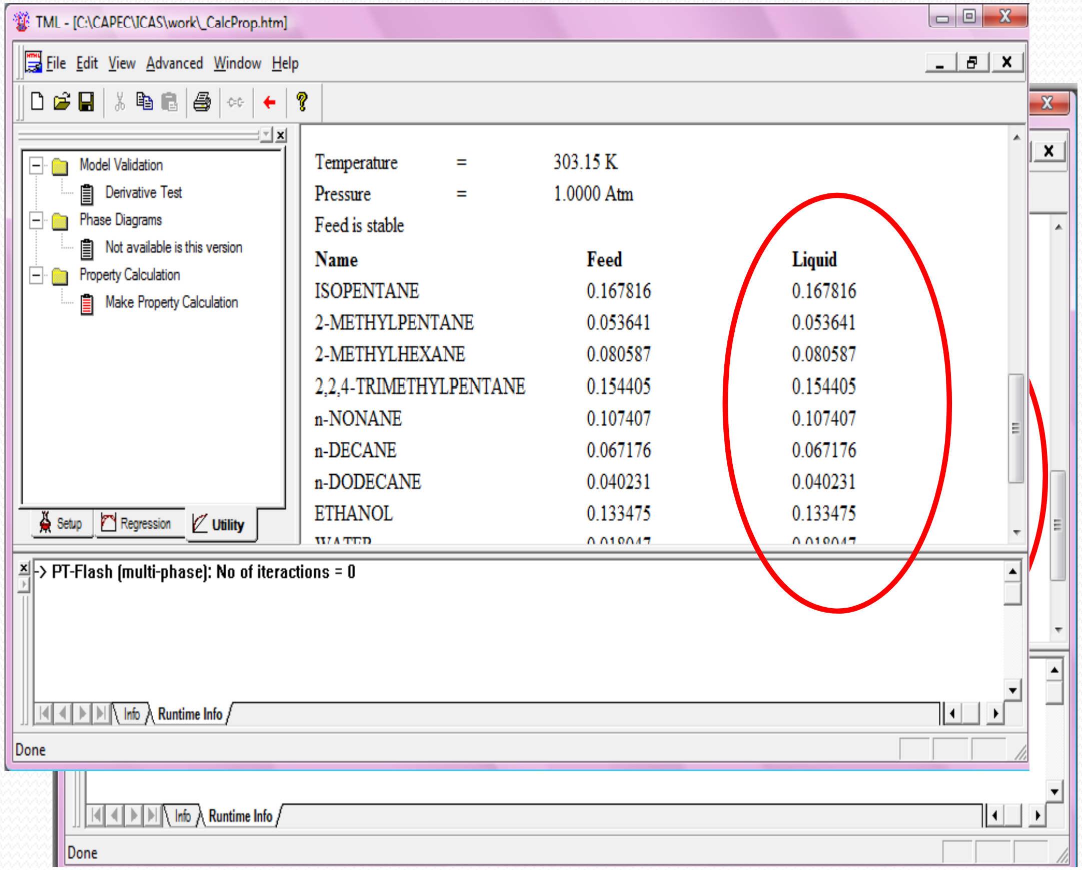

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Methodology

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Using GAMS (General Algebraic Modeling System)

Property constraint:

$HV = \sum x_i HV_i$

$ON = \sum x_i ON_i$

$\rho_{mix} = \sum x_i \rho_i$

$v_{mix} = \frac{1}{\rho_{mix}} \exp\left(\sum \upsilon_i \ln \eta_i\right)$

Volume constraint

$V_{gasoline} \geq 0.5$

$V_{ethanol} \leq 0.05$

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Methodology

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Target Properties	ρ (kg/m^3)	ν (mm^2/s)	HHV (KJ/kg)	Wt % O_2	ON
Gasoline	686.85	0.71	48028	0.00	95
Ethanol	769.84	1.84	29136	34.00	110
Butanol	805.89	3.15	36212	21.60	102.74
MTHF	808.20	0.36	36059	18.57	112.2

Methodology

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Future work

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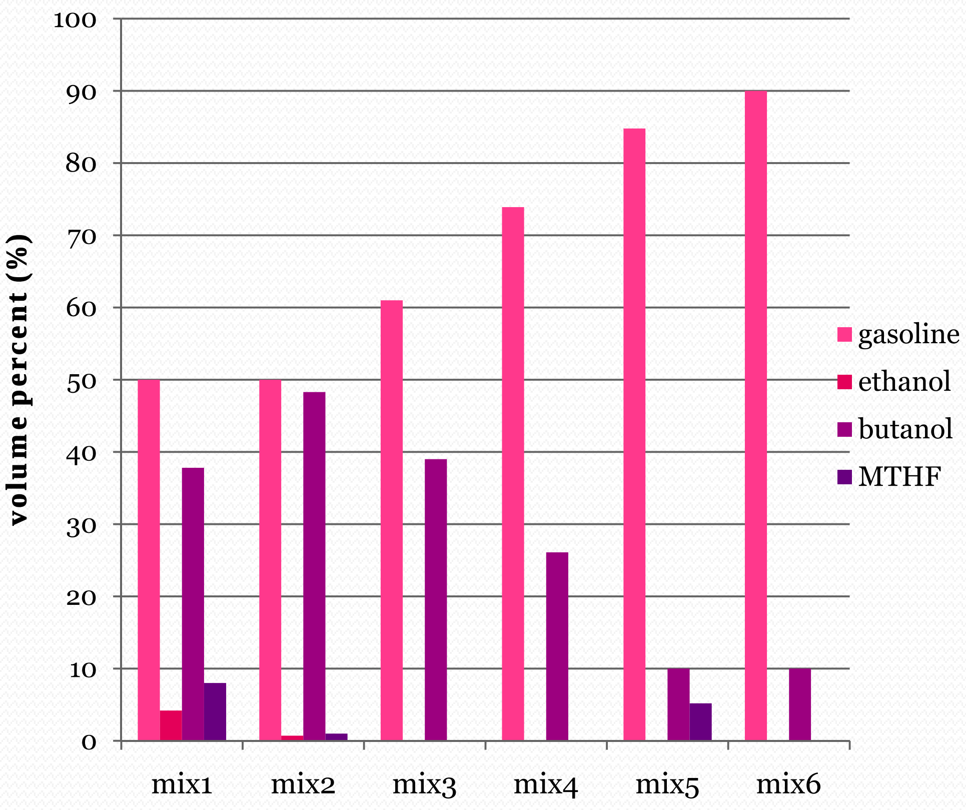
Results

Composition	Mix 1	Mix2	Mix3	Mix4	Mix5	Mix6
Gasoline	0.500	0.500	0.610	0.739	0.848	0.90
Ethanol	0.042	0.007				
Butanol	0.378	0.483	0.390	0.261	0.100	0.10
MTHF	0.08	0.010			0.052	
Property						
HV	41.167	41.473	42.779	44.414	45.945	46.746
Density	749.156	749.130	736.186	720.522	707.696	700.000
Viscosity	0.00152	0.00174	0.0016	0.00138	0.00106	0.00109
ON	100	99	98	97	96	95

Results



- All candidates consist of butanol
- Butanol is most favorable component due to attractive characteristics
- It has higher energy content which is close to gasoline energy content, less prone to water contamination and less corrosive

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Conclusion

- A systematic computer aided technique is a resources efficient technique which is suitable to find a set of target candidates
- Property model availability is one of the challenges in chemical product design

Future work

- Including emission factor to produce a green fuel
- Model validation through a series of experimental work

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THANK YOU
Q&A session